ABSTRACT OF THE DISCLOSURE

A method of introducing conjugated caps onto molecular fragments is described. A first molecule may be decomposed or cut into molecular fragments. Molecular caps may then be introduced in the form of conjugated caps onto the molecular fragments at the decomposition points to form molecular portions. The interaction energy between the molecular portion and a second molecule can then be calculated. This scheme, termed molecular fractionation with conjugated caps, makes it possible and practical to carry out full quantum mechanical (ab initio) calculation of intermolecular interaction energies involving molecules, such as proteins or other biological molecules.